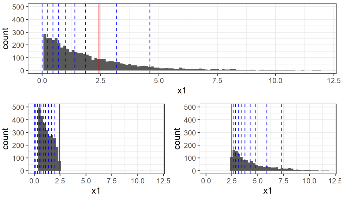
Introduction to Machine Learning

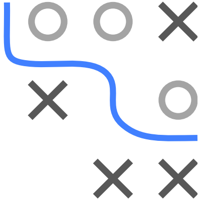
Gradient Boosting: Deep Dive XGBoost Optimization



Learning goals

- Understand details of the regularized risk in XGBoost
- Understand approximation of loss used in optimization
- Understand split finding algorithm

RISK MINIMIZATION



XGBoost uses a risk function with 3 regularization terms:

$$\mathcal{R}_{\text{reg}}^{[m]} = \sum_{i=1}^{n} L\left(y^{(i)}, f^{[m-1]}(\mathbf{x}^{(i)}) + b^{[m]}(\mathbf{x}^{(i)})\right) + \lambda_1 J_1(b^{[m]}) + \lambda_2 J_2(b^{[m]}) + \lambda_3 J_3(b^{[m]}),$$

with $J_1(b^{[m]}) = T^{[m]}$ the number of leaves in the tree to penalize tree depth.

$J_2(b^{[m]}) = \left\|\mathbf{c}^{[m]}\right\|_2^2$ and $J_3(b^{[m]}) = \left\|\mathbf{c}^{[m]}\right\|_1$ are $L2$ and $L1$ penalties of the terminal region values $c_t^{[m]}, t = 1, \dots, T^{[m]}$.

We define $J(b^{[m]}) := \lambda_1 J_1(b^{[m]}) + \lambda_2 J_2(b^{[m]}) + \lambda_3 J_3(b^{[m]})$.

RISK MINIMIZATION

To approximate the loss in iteration m, a second-order Taylor expansion around $f^{[m-1]}(\mathbf{x})$ is computed:

$$
\begin{aligned}
L(y, f^{[m-1]}(\mathbf{x}) + b^{[m]}(\mathbf{x})) \approx \\
L(y, f^{[m-1]}(\mathbf{x})) + g^{[m]}(\mathbf{x}) b^{[m]}(\mathbf{x}) + \frac{1}{2} h^{[m]}(\mathbf{x}) b^{[m]}(\mathbf{x})^2,
\end{aligned}
$$

with gradient

$$
g^{[m]}(\mathbf{x}) = \frac{\partial L(y, f^{[m-1]}(\mathbf{x}))}{\partial f^{[m-1]}(\mathbf{x})}
$$

and Hessian

$$
h^{[m]}(\mathbf{x}) = \frac{\partial^2 L(y, f^{[m-1]}(\mathbf{x}))}{\partial f^{[m-1]}(\mathbf{x})^2}.
$$

Note: $g^{[m]}(\mathbf{x})$ are the negative pseudo-residuals $-\tilde{r}^{[m]}$ we use in standard gradient boosting to determine the direction of the update.

RISK MINIMIZATION

Since $L(y, f^{[m-1]}(\mathbf{x}))$ is constant, the optimization simplifies to

$$
\begin{aligned}
\mathcal{R}_{\text{reg}}^{[m]} &= \sum_{i=1}^{n} g^{[m]}(\mathbf{x}^{(i)}) b^{[m]}(\mathbf{x}^{(i)}) + \frac{1}{2} h^{[m]}(\mathbf{x}^{(i)}) b^{[m]}(\mathbf{x}^{(i)})^2 + J(b^{[m]}) + const \\
&\propto \sum_{t=1}^{T^{[m]}} \sum_{\mathbf{x}^{(i)} \in R_t^{[m]}} g^{[m]}(\mathbf{x}^{(i)}) c_t^{[m]} + \frac{1}{2} h^{[m]}(\mathbf{x}^{(i)}) (c_t^{[m]})^2 + J(b^{[m]}) \\
&= \sum_{t=1}^{T^{[m]}} G_t^{[m]} c_t^{[m]} + \frac{1}{2} H_t^{[m]} (c_t^{[m]})^2 + J(b^{[m]}).
\end{aligned}
$$

Where $G_t^{[m]}$ and $H_t^{[m]}$ are the accumulated gradient and Hessian values in terminal node t.

RISK MINIMIZATION

Expanding $J(b^{[m]})$:

$$
\begin{aligned}
\mathcal{R}_{\text{reg}}^{[m]} &= \sum_{t=1}^{T^{[m]}} \left(G_t^{[m]} c_t^{[m]} + \frac{1}{2} H_t^{[m]} (c_t^{[m]})^2 + \frac{1}{2} \lambda_2 (c_t^{[m]})^2 + \lambda_3 |c_t^{[m]}| \right) + \lambda_1 T^{[m]} \\
&= \sum_{t=1}^{T^{[m]}} \left(G_t^{[m]} c_t^{[m]} + \frac{1}{2} (H_t^{[m]} + \lambda_2)(c_t^{[m]})^2 + \lambda_3 |c_t^{[m]}| \right) + \lambda_1 T^{[m]}.
\end{aligned}
$$

Note: The factor $\frac{1}{2}$ is added to the *L*2 regularization to simplify the notation as shown in the second step. This does not impact estimation since we can just define $\lambda_2 = 2\tilde{\lambda}_2$.

RISK MINIMIZATION

Computing the derivative for a terminal node constant value $c_t^{[m]}$ yields

$$\frac{\partial \mathcal{R}_{\text{reg}}^{[m]}}{\partial c_t^{[m]}} = (G_t^{[m]} + \operatorname{sign}(c_t^m)\lambda_3) + (H_t^{[m]} + \lambda_2)c_t^m.$$

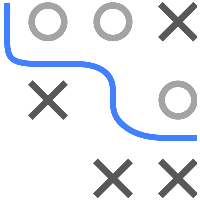
The optimal constants $\hat{c}_1^{[m]}, \dots, \hat{c}_{T^{[m]}}^{[m]}$ can then be calculated as

$$\hat{c}_t^{[m]} = -\frac{t_{\lambda_3}\left(G_t^{[m]}\right)}{H_t^{[m]} + \lambda_2}, t = 1, \dots T^{[m]},$$

with

$$t_{\lambda_3}(x) = \begin{cases} x + \lambda_3 & \text{for } x < -\lambda_3 \\ 0 & \text{for } |x| \leq \lambda_3 \\ x - \lambda_3 & \text{for } x > \lambda_3. \end{cases}$$

LOSS MINIMIZATION - SPLIT FINDING



To evaluate the performance of a candidate split that divides the instances in region $R_t^{[m]}$ into a left and right node we use the **risk reduction** achieved by that split:

$$\tilde{S}_{LR} = \frac{1}{2}\left[\frac{t_{\lambda_3}\left(G_{tL}^{[m]}\right)^2}{H_{tL}^{[m]} + \lambda_2} + \frac{t_{\lambda_3}\left(G_{tR}^{[m]}\right)^2}{H_{tR}^{[m]} + \lambda_2} - \frac{t_{\lambda_3}\left(G_{t}^{[m]}\right)^2}{H_{t}^{[m]} + \lambda_2}\right] - \lambda_1,$$

where the subscripts L and R denote the left and right leaves after the split.

LOSS MINIMIZATION - SPLIT FINDING

Algorithm (Exact) Algorithm for split finding

```
Input I: instance set of current node
Input p: dimension of feature space
gain ← 0
G ← Σ_{i∈I} g(x^(i)), H ← Σ_{i∈I} h(x^(i))
for j = 1 → p do
    G_L ← 0, H_L ← 0
    for i in sorted(I, by x_j) do
        G_L ← G_L + g(x^(i)), H_L ← H_L + h(x^(i))
        G_R ← G − G_L, H_R ← H − H_L
        compute S̃_LR
    end for
end for
Output Split with maximal S̃_LR
```

Input I: *instance set of current node*

Input p: *dimension of feature space*

gain $\leftarrow 0$

$G \leftarrow \sum_{i \in I} g(\mathbf{x}^{(i)})$, $H \leftarrow \sum_{i \in I} h(\mathbf{x}^{(i)})$

for $j = 1 \rightarrow p$ **do**

  $G_L \leftarrow 0$, $H_L \leftarrow 0$

  for i in sorted(I, by x_j) **do**

    $G_L \leftarrow G_L + g(\mathbf{x}^{(i)})$, $H_L \leftarrow H_L + h(\mathbf{x}^{(i)})$

    $G_R \leftarrow G - G_L$, $H_R \leftarrow H - H_L$

    compute $\tilde{S}_{LR}$

  end for

end for

Output Split with maximal $\tilde{S}_{LR}$